Opinion Article

# The Benefits and Challenges with Recent Work in Molecular Catalysis

## Christensen Jensen\*

Department of Molecular Catalysis, Technical University of Denmark, Lyngby, Denmark

#### DESCRIPTION

## Molecular catalysis

Molecular catalysis is not a well-defined field but it always refers to associate application of molecular chemistry, significantly molecular recognition and guest binding, toward chemical action. The ability to target a specific section of a molecule for a reaction makes it easier to make more complicated compounds with several reactive groups.

The extremely programmable nature of molecular catalysts, with varied features that can be precisely regulated, is one of the main advantages. Many metal-centered catalysts have multiple ligands that can all be changed to change the reactivity. These ligands can be totally replaced with a different molecule or slightly modified with a base structure that is comparable. The metal center can also be changed, and the same set of ligands can be used on other metals or in different oxidation states of the same metal. Researchers may now compare reactivity and see how changes in a variety of chemical and physical parameters affect catalysis.

Working with molecular catalysts also has the advantage of being amenable to a variety of analytical techniques that allow for thorough observations of the catalytic process. Researchers can use these small-molecule-targeted techniques to discover reactions and intermediates, as well as assess the catalyst's success. Examining the reaction processes in depth allows researchers to gain a better knowledge of how catalysts work, as well as insight into how to change catalysts to produce more efficient reactions.

### Challenges

The scope of molecular catalysis must be limited to molecular systems with all components being molecules. When compared to solid-phase catalysts, these molecular systems show problems. When everything is dissolved in the same solution, separating the catalyst from the rest of the reaction mixture can be a significant challenge. Purification to separate the products from the catalyst is generally time-consuming and costly. It's very

crucial to keep it separate from the reaction mixture. Metals like ruthenium, iridium, and platinum, which are extremely scarce and expensive, are used in many metal-containing molecular catalysts. The production of highly engineered catalysts can take a long time and demand making them difficult to come by. The stability of molecular catalysts is also a drawback. Solid-phase catalysts are often used at high temperatures, but molecular catalysts deteriorate at temperatures as low as 100°C. Significant research has resulted in more stable molecular catalysts that can work at temperatures nearly 200°C, however only a small number of catalysts have this level of thermal stability. Deactivation of catalysts can occur as a result of interactions with substances that are accidentally present in the mixture, such as oxygen or reaction side products. Deactivation, often known as poisoning, is a problem that affects all types of catalysts and necessitates avoiding.

The manufacture of usable products, "solar fuels," in which solar energy would be stored, is the fundamental goal of recent attention generated by the decrease of carbon dioxide. Designing photochemical methods that operate this conversion using directly solar light energy is one path to this goal. An indirect strategy is first converting sunshine energy into electricity and then electrochemically reducing CO2. Carbon dioxide to carbon monoxide conversion is thus a crucial step in the conventional dihydrogen-reductive Fischer-Tropsch synthesis. Overall, it appears that iron porphyrins are not only the most efficient catalysts for the CO2-to-CO electrochemical conversion, but they may also be used to show broader difficulties in the field of molecular catalysis, such as other reductive or oxidative reactions.

#### Recent work in molecular catalysis

Much of the early studies in molecular catalysis relied on rare metals, which are in short supply on Earth. Although these elements have features that make them useful as catalyst centres, current attempts have pushed the sector to use more Earthabundant metals. This effort has resulted in further research into metals including nickel, copper, and iron. Different ligands, in addition to new metal centers, are required to fully harness the promise of these compounds as efficient catalysts. As a

Correspondence to: Dr. Christensen Jensen, Department of Molecular Catalysis, Technical University of Denmark, Lyngby, Denmark, E-mail: jensench@live.com

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result, research has shifted to more complex ligands. These meticulously constructed compounds undergo lengthy syntheses and are finely tuned to exhibit desired features. This tuning can be done from a steric standpoint, as ligand size effects how substrates attach to the catalyst, or from an electronic standpoint, as ligands can add or remove electron density at the metal center in an organometallic complex. Ligands are frequently more than bystanders in the presence of a catalytically active metal core, and they can work together to impact catalysis. Metal-ligand collaboration, also known as metal-ligand cooperation is a growing topic.

Some ligands are made to bind two metals instead of just one. The resulting bimetallic species can catalyse more complex processes by combining the characteristics of various metals, which can be the same or different. A bimetallic catalyst, for example, can have two active sites that connect to separate substrates and keep them close together. Alternatively, the two metals can form associations with separate parts of the same substrate to boost the molecule's overall reactivity and activate a particularly difficult target.